CHBE 505
Advanced Numerical Methods

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Office: B235 Abercrombie
Class Room: TBD

Class Hours: 9:25 AM –10:40 AM (T, Th)
Office Hours: TBD

Teaching assistants

TBD

Course Description

Modern engineering practice and scientific research is increasingly reliant on scientific computing. Thus it is imperative that the graduate student be (a) proficient in numerical methods and (2) in their computer implementation. Programming literacy is indispensable in implementing computational methods; it encompasses the both proficiency in the programming language and in computational thinking, an aspect that is independent of the programming language and is a skill that is broadly applicable to all problem solving and analysis.

The focus of this course is on numerical methods and their computational implementation. In this course, depending on your prior programming expertise, you are encouraged to either use MATLAB or Python. Please note that MATLAB is available for no-cost to Rice students. Python is a high level interpreted language that is distributed free on the internet. The Anaconda Python distribution also automatically gives you access to extensive libraries for numerical methods and visualization.

Course Objectives

1. Linear Algebraic Systems
2. Nonlinear Algebraic Systems
3. Initial Value Problems
4. Boundary Value Problems
5. Probability theory and Stochastic Methods
6. Numerical Optimization (if time permits)
7. Fourier Methods (if time permits)

Required Textbook

- Numerical Methods with Chemical Engineering Applications by Kevin Dorfman and Prodromos Daoutidis
  - This is an undergraduate level text, but is also suitable for a beginning graduate student.
  - This text does not cover Stochastic Methods and Numerical Optimization. For those parts we will rely on class notes.

Supplemental Reading

- Numerical Methods for Chemical Engineering — Applications in MATLAB by Kenneth Beers
  - This is a graduate-level text and besides the topics covered in the class text it includes chapters on Stochastic Methods and Optimization.
- Numerical Recipes: The art of scientific computing by Press, Teukolsky, Vellerling, and Flannery.
  - This fantastic book provides an exhaustive tour of numerical methods. The implementation of methods is discussed in detail and code is provided for different languages, such as Fortran and C. A must have book for any researcher / engineer who expects to do extensive numerical work.
- Class Notes
  - Students should have a copy of the class text; class notes will be posted as and when necessary.

Course Organization

We will discuss the organization in detail in the class and will post the plan by the end of week # 1.

- The course will comprise four (4) assignments which will be designated as non-pledged (see Honor code policy below)
- Two (2) assignments will be pledged (see Honor code policy below)

Please note that while we encourage the use of MATLAB or Python, students who are proficient in a lower level language such as C++ or Fortran are free to use that. But given our constraints, we will be unable to provide specific language-related help in these cases.

Honor code Policy

Students are encouraged to talk to each other, the teaching assistants, the instructor, or anyone else about any assignment in the course that is not specifically designated as pledged. For assignments that are pledged, you can **only discuss with the instructor and/or TAs**; you cannot consult any other resource (excluding programming language specific help files). For all assignments, consulting another student's solution is prohibited. Your submissions should not be copied from any source.

ADA Statement

Any student with a documented disability needing academic adjustments or accommodations is requested to speak with the instructor during the **first two weeks of class**. All discussions will remain confidential. Students with disabilities will need to also contact Disability Support Services in the Allen Center.

Grading Policy

Grade	%
Non-pledged assignments	60
Pledged assignments	40

Late assignments will incur a penalty of 20% / day after the submission deadline.
Provisionally, we plan to follow the distribution below in assigning letter grades. Reasonable adjustments will be made if the average drops much below our expectation.

Grade	%
A+	≥ 98
A	$92.0 - 97.9$
A-	$86.0 - 91.9$
B+	$80.0 - 85.9$
B	$70.0 - 79.9$
B-	$60.0 - 69.9$
C	< 59.9